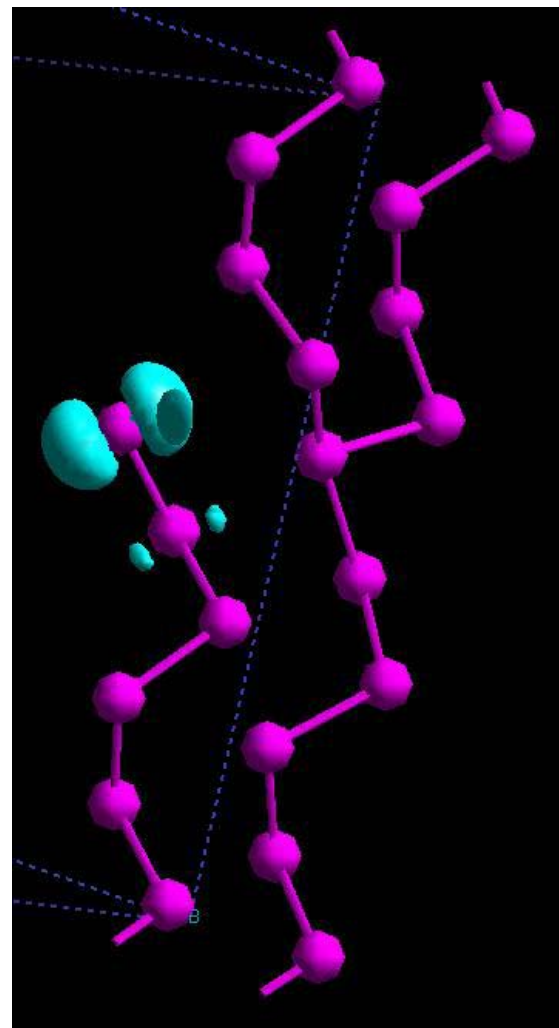


# Theory of Non-crystalline solids, D. A. Drabold, Ohio University, DMR 0310933

Amorphous selenium is used for digital X-ray radiography, xerography and other applications. Here we show a “valence alternation pair” defect and an unpaired spin density (blue) with pink Se atoms. Such defects limit performance in applications. A first principles local spin-density calculation was employed with realistic models. This illustration was employed on the cover of a 2003 book published by Wiley.



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**Education:** Three PhD students and a postdoctoral associate are fully or partly funded by this award. Two of our recent DMR-funded graduates (Dong and Durandurdu) are in tenure track positions at Auburn and the University of Texas, El Paso.

**Broader Impacts:** We are working with a small company (Axon Technologies on Tempe, AZ) on column VI binary chalcogenide (germanium selenide) glasses alloyed with silver to develop an improved computer memory device. We co-organized an international workshop (M. F. Thorpe Festschrift) with topics ranging from biophysics to Hubbard models, and edited the proceedings.



Partial Group photo: D. Tafen (student), visitor P. Ordejon, Drabold, R. Atta-Fynn (student), P. Biswas(post-doc)